Numerical Solutions of Coupled Thermo-Mechanical Problems with Applications in Geomechanics

Nedoma, Jiří
2001

Institute of Computer Science
Academy of Sciences of the Czech Republic

Numerical Solutions of Coupled Thermo-Mechanical Problems with Applications in Geomechanics

Jiří Nedoma

Technical report No. 822

March 2001

Pod Vodárenskou věží 2, 182 07 Prague 8, phone: (+4202) 6605 1111, fax: (+4202) 858 57 89,
e-mail:nedoma@cs.cas.cz

Institute of Computer Science
Academy of Sciences of the Czech Republic

Numerical Solutions of Coupled Thermo-Mechanical Problems with Applications in Geomechanics

Jiří Nedoma

Technical report No. 822

March 2001

Abstract:

Temperature plays an important role in geomechanics as it strongly controls the rheology of the rocks. The main intrinsic rheological parameters affecting the mechanical behaviour of materials are time, temperature and pressure, as well as chemical environment (diffusion). Many geomechanical processes connected with heat and diffusion involving phase-change phenomena lead to solving free boundary problems of the two-phase Stefan-like type. Therefore mathematical simulations of thermo-mechanical processes play an important role to better understand the resulting rock behaviour.

In the contribution coupled thermo-mechanical processes based on the theory of contact problems in linear and non-linear thermo-elasticity will be discussed. The geodynamical as well as geomechanical processes connected with the construction of the radioactive waste repositories will be also shortly discussed.

Keywords:
Thermo-mechanical problems, heat problems, Stefan-like problems, enthalpy formulation, contact problems with friction, variational inequalities, finite element approximation, thermo-elasticity, thermo-visco-plasticity, geomechanics, radioactive waste repositories.

1 Introduction

The heat in the rock massif is transferred by conduction. The thermo-mechanical analyses are very important in regions where e.g. radioactive waste repositories will be situated. The temperature field can be determined by solving the relevant form of heat conduction equation and the stress-strain field by solving the contact problem. Many geomechanical processes connected with heat flow and diffusion involving phase-change phenomena give rise to free boundary problems for parabolic partial differential equations of the two-phase Stefan type.

Since the geothermal and geomechanical processes are connected, the mathematical models describing single geomechanical processes in the upper part of the Earth must be derived from the global geomechanical model. Therefore we will shortly illustrate the global evolutionary mathematical model and in more details we will present mathematical models which can be (and were) used for investigation of plate tectonic and geomechanical models under the presumption that the geological time period is relatively short and that the invasing plate during the assumed time period moves at a constant speed or that the geomechanical process can be investigated as a static problem. Since the motion of the invasing plate is divided into relatively small time steps and the rock properties behave for such time periods elastically, then the models can be described by the semi-coercive contact problems in (non-)linear elasticity.

2 Mathematical Problems in Coupled Thermo-Mechanics

We will assume that the geological bodies are of arbitrary shapes and, moreover, are in mutual contacts. On the Earth boundary the geological bodies are loaded while on the remaining part of the investigated region we estimate the effect of movement (if it exists) of the invasing geological body in time. Therefore, as a result, some geological bodies can shift and rotate. Such problems are represented by semi-coercive contact problems.

Further a semi-coercive contact problem in non-linear thermo-elastic rheology will be formulated and analysed. For determination of the rheology we develop the N-dimensional stress-strain relation ($N = 2, 3$) derived from the positive definite strain energy density function W of form $W = A_1^{\lambda_1} + A_2^{\lambda_2}(e_{ij}) + A_3^{\lambda_3}(e_{ij})$, where A_1, A_2, A_3 are scalar-valued functions of strains e_{ij} and λ_i, $i = 1, 2, 3$ are positive parameters. We will assume that $\lambda_1 = \lambda$, $\lambda_2 = \lambda_3 = 1$. The parameter λ determines the degree of non-linearity for the strain dependent anisotropic elasto-plastic coefficients, which are functions of the displacement vector $\mathbf{u}$ and temperature T. For $0 < \lambda < 1$ the parameter λ has the effect of producing a softening stress-strain curve, for $\lambda > 1$ it has the effect of producing a hardening strain curve. For $\lambda = 1$ it produces strain-less elastic curves, where the non-linearity follows from the anisotropic coefficients depending on the displacement $\mathbf{u}$ and temperature T only.

For the derivation of the geomechanical model, we first derive the global evolutionary model and then, on its basis, the local geomechanical models will be derived.

To develop the N-dimensional stress-strain relation ($N = 2, 3$) a positive definite strain energy density function will be used. Let the strain energy density function W be defined by

$$W = A_1^{\lambda}(e_{ij}) + A_2(e_{ij}) + A_3(e_{ij}) \,, \tag{2.1}$$

where $A_i, i = 1, 2, 3$, are scalar-valued functions of the strains e_{ij} and λ is a positive parameter (Fung, 1965). In this paper we will assume that functions A_1, A_2, A_3 are defined as

$$\begin{aligned} A_1 &= c_{ijkl}(\mathbf{u})e_{ij}(\mathbf{u})e_{kl}(\mathbf{u}) \,, \qquad A_2 = C_{ijkl}e_{ij}(\mathbf{u})e_{kl}(\dot{\mathbf{u}}) \,, \\ A_3 &= -\beta_{ij}(T - T_0)e_{ij}(\mathbf{u}) \,, \qquad e_{ij}(\mathbf{u}) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \; i,j,k,l = 1,\ldots,N, \end{aligned} \tag{2.2}$$

where e_{ij} is a small strain tensor, c_{ijkl} are elasto-plastic coefficients generally depending on the displacement vector $\mathbf{u} = (u_i)$, C_{ijkl} are viscous coefficients also depending on coordinates $\mathbf{x}$, β_{ij} are thermal expanding coefficients depending on the coordinates $\mathbf{x}$. Assume that

$$c_{ijkl} = c_{klij} = c_{jikl}\,,\ \ C_{ijkl} = C_{klij} = C_{jikl}\,,\ \ \beta_{ij} = \beta_{ji}\,.$$

A repeated index implies summation from 1 to N. According to the theory of continuum mechanics and thermodynamics the stress tensor components are defined by the well-known relation

$$\tau_{ij} = \frac{\partial W}{\partial e_{ij}}\,. \tag{2.3}$$

Hence and using (2.2)

$$\begin{aligned}
\tau_{ij} &= \lambda[A_1(e_{ij})]^{\lambda-1}\frac{\partial A_1(e_{ij})}{\partial e_{ij}} + \frac{\partial A_2(e_{ij})}{\partial e_{ij}} + \frac{\partial A_3(e_{ij})}{\partial e_{ij}} = \\
&= 2\lambda[A(e_{ij})]^{\lambda-1}c_{ijkl}(\mathbf{u})e_{kl}(\mathbf{u}) + C_{ijkl}e_{kl}(\dot{\mathbf{u}}) - \beta_{ij}(T-T_0) = \\
&= c^*_{ijkl}(\mathbf{u})e_{kl}(\mathbf{u}) + C_{ijkl}e_{kl}(\dot{\mathbf{u}}) - \beta_{ij}(T-T_0)\,.
\end{aligned} \tag{2.4}$$

The scalar coefficient $2\lambda[A_1(e_{ij})]^{\lambda-1}$ depends upon the state of strain and can simulate hardening and softing behaviours of materials. Then

$$c^*_{ijkl}(\mathbf{u}) = 2\lambda[A_1(e_{ij})]^{\lambda-1}c_{ijkl}(\mathbf{u}) \tag{2.5}$$

are strain dependent non-linear elastic coefficients. Parameter λ determines the degree of non-linearity for the strain dependent elasto-plastic coefficients $c^*_{ijkl}(\mathbf{u})$. If $\lambda < 1$ then the parameter λ has the effect of producing a softening stress-strain curve, if $\lambda = 1$ it produces the strain-less elastic curve where the non-linear coefficients $c^*_{ijkl}(\mathbf{u})$ depend on the displacements $\mathbf{u}$ only, while for $\lambda > 1$ it has the effect of producing a hardening stress-strain curve. The viscous term with short memory $C_{ijkl}(\mathbf{x})e_{kl}(\dot{\mathbf{u}})$ can be changed by the viscous term with long memory (see e.g. Freudenthal and Geiringer, 1958; Duvaut and Lions, 1976), i.e. by $\sum_{m=1}^{n} C^m_{ijkl}(\mathbf{x})\frac{\partial^m}{\partial t^m}e_{kl}(\mathbf{u}) + \int_0^t b_{ijkl}(t-\tau)e_{kl}(\mathbf{u})d\tau$ for the so-called materials of "rate type" or in a simple form by $C_{ijkl}(\mathbf{x})e_{kl}(\dot{\mathbf{u}}) + \int_0^t b_{ijkl}(t-\tau)e_{kl}(\mathbf{u})d\tau$. Moreover, phase transition zones can be also studied. For such a problem the Stefan-like conditions on the phase change boundaries (see e.g. Nedoma, 1998) must be defined.

The model

Let $\Omega \subset R^N$ be a region occupied by a system of elasto-visco-plastic bodies Ω^ι, so that $\Omega = \bigcup_{\iota=1}^{s}\Omega^\iota$. Let Ω^ι have Lipschitz boundaries $\partial\Omega^\iota$ and assume that $\partial\Omega = \Gamma_\tau \cup \Gamma_u \cup \Gamma_c \cup \Gamma_0 \cup \mathcal{R}$, where the disjoint parts Γ_τ, Γ_u, Γ_c and Γ_0 are open subsets and the surface measure of $\mathcal{R}$ is zero. Moreover, let $\Gamma_u =^1 \Gamma_u \cup\ ^2\Gamma_u$ and $\Gamma_c^{kl} = \partial\Omega^k \cap \partial\Omega^l$, $k \neq l$, $\overline{\Gamma}_c = \bigcup_{k,l}\Gamma_c^{kl}$.

Let $u_n = u_i n_i$, $\mathbf{u}_t = \mathbf{u} - u_n\mathbf{n}$, $\tau_n = \tau_{ij}n_j n_i$, $\boldsymbol{\tau}_t = \boldsymbol{\tau} - \tau_n\mathbf{n}$ be normal and tangential components of displacement and stress vectors $\mathbf{u} = (u_i), \boldsymbol{\tau} = (\tau_i)$, $\tau_i = \tau_{ij}n_j$, $i,j = 1,\ldots,N$, $\mathbf{n} = (n_i)$ is the unit outward normal vector to $\partial\Omega$.

Let body forces $\mathbf{F} \in [L^2(\Omega)]^N$, surface forces $\mathbf{P} \in [L^2(\Gamma_\tau)]^N$ and slip limits $g_c^{kl} \in [L^2(\Gamma_c^{kl})]^N$ be given. Then the model to be solved represents a contact problem in non-linear thermo-elasto-visco-plasticity. For the derivation of contact conditions see e.g. Nedoma (1998). Then the global model is as follows:

Global Model Problem:

Let $N = 2(3)$, $s \geq 2$. Find a pair of functions $(T, \mathbf{u})$, scalar function T and vector function $\mathbf{u}$, satisfying

$$c^\iota \frac{\partial T^\iota}{\partial t} + \rho^\iota \beta^\iota_{ij} T^\iota_0 e_{ij}(\dot{\mathbf{u}}^\iota) - \frac{\partial}{\partial x_i}\left(\kappa^\iota_{ij}\frac{\partial T^\iota}{\partial x_j}\right) = W^\iota, \;\; \rho^\iota \frac{\partial^2 u^\iota_i}{\partial t^2} = \frac{\partial \tau_{ij}(\mathbf{u}^\iota)}{\partial x_j} + F^\iota_i,$$
$$i,j = 1,\dots,N,\; \iota = 1,\dots,s \;\text{ in } \Omega^\iota\,, \tag{2.6}$$
$$\tau^\iota_{ij} = c^{*\iota}_{ijkl}(\mathbf{u}^\iota)e_{kl}(\mathbf{u}^\iota) + C^\iota_{ijkl}e_{kl}(\dot{\mathbf{u}}^\iota) - \beta^\iota_{ij}(T^\iota - T^\iota_0), \quad i,j,k,l = 1,\dots,N,\; \iota = 1,\dots,s\,, \tag{2.7}$$
$$T = T_1,\; \tau_{ij}n_j = P_i, \quad i,j = 1,\dots,N \;\text{ on } \Gamma_\tau\,, \tag{2.8}$$
$$\kappa_{ij}\frac{\partial T}{\partial x_j}n_i = 0,\; u_i =^1 u_{0i}, \quad i,j = 1,\dots,N \;\text{ on } {}^1\Gamma_u\,, \tag{2.9}$$
$$T = T_2 \;\left(\text{or } \kappa_{ij}\frac{\partial T}{\partial x_j}n_i = q_0\right),\; u_i =^2 u_{0i}, \quad i = 1,\dots,N, \;\text{ on } {}^2\Gamma_u\,, \tag{2.10}$$
$$T^k = T^l,\; \kappa_{ij}\frac{\partial T}{\partial x_i}n_{i|(k)} = \kappa_{ij}\frac{\partial T}{\partial x_i}n_{i|(l)} \;\text{ on } \Gamma^{kl}_c\,, \tag{2.11}$$
$$u^k_n - u^l_n \le 0,\; \tau^k_n = -\tau^l_n \equiv \tau^{kl}_n \le 0,\; (u^k_n - u^l_n)\tau^{kl}_n = 0 \;\text{ on } \Gamma^{kl}_c\,, \tag{2.12}$$
$$\text{if } u^k_n - u^l_n = 0 \text{ then } |\tau^{kl}_t| \le g^{kl}_c \;\text{ on } \Gamma^{kl}_c\,, \tag{2.13}$$
and
$$\text{if } \mid \boldsymbol{\tau}^{kl}_t \mid < g^{kl}_c \text{ then } \mathbf{u}^k_t - \mathbf{u}^l_t = 0\,, \tag{2.14}$$
$$\text{if } \mid \boldsymbol{\tau}^{kl}_t \mid = g^{kl}_c \text{ then there exists a function } \vartheta \ge 0 \text{ such that } \mathbf{u}^k_t - \mathbf{u}^l_t = -\vartheta \boldsymbol{\tau}^{kl}_t\,, \tag{2.15}$$

where c^ι is the heat capacity, $\rho^\iota \beta^\iota_{ij} T^\iota_0 e_{ij}(\mathbf{u}^{\iota\prime})$ represents the dissipative deformation energy changing into heat, T_1, T_2 are given temperatures, q_0 is a given heat flow. On part Γ_0 of boundary $\partial\Omega$, representing the condition of symmetry or the condition for useful limitation of the investigated (namely of 3D) region, we can use conditions

$$u_n = 0,\; \tau_{tj} = 0, \quad j = 1,\dots,N \;\text{ on } \Gamma_0 \tag{2.16}$$

It is evident that such problems are very difficult for detailed analyses. Therefore, in the next part we will limit ourselves to simple model problems for which parameter $\lambda = 1$.

2.1 Coupled Thermo-Mechanical Models

Introduction

In mechanics and geomechanics there is a variety of variational formulations. Variational inequalities physically describe the principle of virtual work in its inequality form. Such problems are represented by contact problems with or without friction in linear elasticity, thermo-elasticity, plasticity and thermo-plasticity (see e.g. Nečas, Hlaváček (1981), Haslinger et al. (1996), Hlaváček et al. (1988), Kikuchi, Oden (1988), Panagiotopoulos (1985) in elasticity and plasticity and Nedoma (1983), (1987), (1994), (1997), (1998) in thermo-elasticity. In Hlaváček, Nedoma (2001) and Nedoma, Hlaváček (2001) we analyse generalized semi-coercive contact problems with friction in static linear and non-linear thermo-elasticity for the case that bodies of arbitrary shapes, being in a mutual contact, are loaded by external forces.

The Model Problem in Non-Linear Rheology

Let $\Omega \subset R^N$ be a region occupied by a system of elastic bodies Ω^ι, so that $\Omega = \bigcup_{\iota=1}^{s} \Omega^\iota$. Let Ω^ι have a Lipschitz boundary $\partial\Omega^\iota$ and assume that $\partial\Omega = \Gamma_\tau \cup \Gamma_u \cup \Gamma_c \cup \mathcal{R}$, where the disjoint parts Γ_τ, Γ_u and Γ_c are open subsets and the surface measure of $\mathcal{R}$ is zero. Moreover, let $\Gamma_u =^1 \Gamma_u \cup {}^2\Gamma_u$ and $\Gamma^{kl}_c = \partial\Omega^k \cap \partial\Omega^l$, $k \ne l$, $\Gamma_c = \bigcup_{k,l} \Gamma^{kl}_c$.

Let $u_n = u_i n_i$, $\mathbf{u}_t = \mathbf{u} - u_n\mathbf{n}$, $\tau_n = \tau_{ij}n_j n_i$, $\boldsymbol{\tau}_t = \boldsymbol{\tau} - \tau_n\mathbf{n}$ be normal and tangential components of displacement and stress vectors $\mathbf{u} = (u_i)$, $\boldsymbol{\tau} = (\tau_i)$, $\tau_i = \tau_{ij}n_j$, $i,j = 1,\dots,N$, $\mathbf{n} = (n_i)$ is the unit outward normal vector to $\partial\Omega$.

Let body forces $\mathbf{F} \in [L^2(\Omega)]^N$, surface forces $\mathbf{P} \in [L^2(\Gamma_\tau)]^N$, displacements $\mathbf{u}_0 \in [W^{1,2}(\Omega)]^N$, slip limits $g^{kl}_c \in [L^2(\Gamma^{kl}_c)]^N$ and a temperature $T_1 = (T_{11}, T_{12}) \in L^2(\Gamma_\tau \cup {}^2\Gamma_2)$ be given. Then the model to be solved represents a contact problem in non-linear thermo-elasticity.

Further, we will investigate the following model problem:

Problem ($\mathcal{P}$): Let $N = 2(3)$, $s \geq 2$. Find a pair of functions $(T, \mathbf{u})$, temperature T and displacement vector $\mathbf{u}$, satisfying

$$-\frac{\partial}{\partial x_i}\left(\kappa_{ij}^{\iota}\frac{\partial T^{\iota}}{\partial x_j}\right) = Q^{\iota}, \quad \frac{\partial \tau_{ij}(\mathbf{u}^{\iota})}{\partial x_j} + F_i^{\iota} = 0, \quad i, j = 1, \ldots, N, \ \iota = 1, \ldots, s \text{ in } \Omega^{\iota}, \tag{2.17}$$

$$\tau_{ij}^{\iota} = c_{ijkl}^{*\iota}(\mathbf{u}^{\iota})e_{kl}(\mathbf{u}^{\iota}) - \beta_{ij}^{\iota}(T^{\iota} - T_0^{\iota}), \ i, j, k, l = 1, \ldots, N, \ \iota = 1, \ldots, s, \tag{2.18}$$

$$T = T_{11}(=0) \ \left(\text{or } \kappa_{ij}\frac{\partial T}{\partial x_j}n_i = 0\right), \ \tau_{ij}n_j = P_i, \ i, j = 1, \ldots, N \text{ on } \Gamma_{\tau}, \tag{2.19}$$

$$\kappa_{ij}\frac{\partial T}{\partial x_j}n_i = 0, \ u_i = {}^1u_{0i}, \ \ i, j = 1, \ldots, N \text{ on } {}^1\Gamma_u, \tag{2.20}$$

$$T = T_{12} \ (\text{or } \kappa_{ij}\frac{\partial T}{\partial x_j}n_i = q_0), \ u_i = {}^2u_{0i}, \ i = 1, \ldots, N, \text{ on } {}^2\Gamma_u, \tag{2.21}$$

$$T^k = T^l, \ \kappa_{ij}\frac{\partial T}{\partial x_j}n_{i|(k)} = \kappa_{ij}\frac{\partial T}{\partial x_j}n_{i|(l)} \text{ on } \Gamma_c^{kl}, \tag{2.22}$$

$$u_n^k - u_n^l \leq 0, \ \tau_n^k = -\tau_n^l \equiv \tau_n^{kl} \leq 0, \ (u_n^k - u_n^l)\tau_n^{kl} = 0 \text{ on } \Gamma_c^{kl}, \tag{2.23}$$

$$\text{if } u_n^k - u_n^l = 0 \text{ then } \ |\boldsymbol{\tau}_t^{kl}| \leq g_c^{kl} \text{ on } \Gamma_c^{kl} \text{ and} \tag{2.24}$$

$$\text{if } \ |\boldsymbol{\tau}_t^{kl}| < g_c^{kl} \text{ then } \mathbf{u}_t^k - \mathbf{u}_t^l = 0, \tag{2.25}$$

$$\text{if } \ |\boldsymbol{\tau}_t^{kl}| = g_c^{kl} \text{ then there exists a function } \vartheta \geq 0 \text{ such that } \mathbf{u}_t^k - \mathbf{u}_t^l = -\vartheta\boldsymbol{\tau}_t^{kl}, \tag{2.26}$$

or in a simple friction-less case

$$\boldsymbol{\tau}_t^{kl} = 0 \text{ on } \Gamma_c^{kl}. \tag{2.27}$$

As our quasi-coupled problem under investigation is not coupled, both the problems in thermics and non-linear elasticity can be solved separately and the coupling term $\frac{\partial}{\partial x_j}(\beta_{ij}^{\iota}(T^{\iota} - T_0^{\iota}))$ has the meaning of body forces.

Let us introduce the sets of virtual temperatures and displacements and the set of admissible displacements by

$$\begin{aligned}
{}^1V &= \left\{z \mid z \in {}^1W \equiv H^1(\Omega^1) \times \cdots \times H^1(\Omega^s), \ z = T_1 \text{ on } \Gamma_{\tau} \cup {}^2\Gamma_u\right\}, \\
V &= \left\{\mathbf{v} \mid \mathbf{v} \in [H^1(\Omega^1)]^N \times \cdots \times [H^1(\Omega^s)]^N, \ \mathbf{v} = \mathbf{u}_0 \text{ on } \Gamma_u\right\}, \\
K &= \left\{\mathbf{v} \mid \mathbf{v} \in V_0, \ v_n^k - v_n^l \leq 0 \text{ on } \bigcup_{k,l}\Gamma_c^{kl}\right\},
\end{aligned}$$

and for detailed analyses the set of all displacements and rotations

$$R^{\iota} = \left\{\mathbf{v} \mid \mathbf{v} \in [H^1(\Omega^{\iota})]^N, \ e_{ij}(\mathbf{v}) = 0 \text{ a.e.}\right\}, \ R = \sqcap_{\iota=1}^s R^{\iota}.$$

For $N = 3$

$$R^{\iota} = \left\{\mathbf{v} \mid \mathbf{v} \in [H^1(\Omega^{\iota})]^3, \ \mathbf{v} = \mathbf{a}^{\iota} + \mathbf{b}^{\iota} \times \mathbf{x}\right\},$$

for $N = 2$

$$R = \left\{\mathbf{v} \mid \mathbf{v} \in [H^1(\Omega^{\iota})]^2, \ v_1 = a_1^{\iota} - b^{\iota}x_2, v_2 = a_2^{\iota} + b^{\iota}x_1\right\},$$

where $\mathbf{a}^{\iota}$, $\mathbf{b}^{\iota}$ are arbitrary real vectors for $N = 3$ or b^{ι} is a real scalar for $N = 2$.

To formulate the variational (weak) formulation of the above problem ($\mathcal{P}$), we multiply (1a) by $z - T$ and (1b) by $v_i - u_i$, integrate over Ω and use boundary conditions. Then after some modifications we obtain the following variational problem:

Find a pair of functions $(T, \mathbf{u})$, $T \in {}^1V$, $\mathbf{u} \in K$, satisfying

$$b(T, z - T) \geq s(z - T) \quad \forall z \in {}^1V_h, \tag{2.28}$$

$$a(\mathbf{u}; \mathbf{u}, \mathbf{v} - \mathbf{u}) \geq (\mathbf{f}, \mathbf{v} - \mathbf{u}) \quad \forall \mathbf{v} \in K, \tag{2.29}$$

where

$$\begin{aligned}
b(T,z) &= \sum_{\iota=1}^{s} b^{\iota}(T^{\iota},z^{\iota}) = \int_{\Omega} \kappa_{ij}(x)\frac{\partial T}{\partial x_j}\frac{\partial z}{\partial x_i}d\mathbf{x}\,,\\
s(z) &= \sum_{\iota=1}^{s} s^{\iota}(z^{\iota}) = \int_{\Omega} Qzd\mathbf{x}\left(+\int_{\Gamma_\tau} q_0 z ds\right),\ l(z) = \frac{1}{2}b(z,z) - s(z)\,,\\
a(\mathbf{w};\mathbf{u},\mathbf{v}) &= \sum_{\iota=1}^{s} a(\mathbf{w}^{\iota};\mathbf{u}^{\iota},\mathbf{v}) = 2\int_{\Omega} \lambda[A(e_{ij}(\mathbf{w}))]^{\lambda-1}c_{ijkl}(\mathbf{w})e_{ij}(\mathbf{u})e_{kl}(\mathbf{v})d\mathbf{x}\,,\\
(\mathbf{f},\mathbf{v}) &= \sum_{\iota=1}^{s}(\mathbf{f}^{\iota},\mathbf{v}) = \int_{\Omega} F_i v_i d\mathbf{x} + \int_{\Gamma_\tau} P_i v_i ds\,.
\end{aligned}$$

For the existence of potential energy functional $L(\mathbf{v})$, such that its Gâteaux differential

$$DL(\mathbf{u},\mathbf{v}) = a(\mathbf{u};\mathbf{u},\mathbf{v}) - (\mathbf{f},\mathbf{v})\,,$$

the following condition is necessary (see e.g. Gajewski et al. (1974)):

$$\int_{\Omega} Dc^{*}_{ijkl}(\mathbf{u},\mathbf{w})e_{kl}(\mathbf{u})e_{ij}(\mathbf{v})d\mathbf{x} = \int_{\Omega} Dc^{*}_{ijkl}(\mathbf{u},\mathbf{v})e_{kl}(\mathbf{u})e_{ij}(\mathbf{w})d\mathbf{x} \quad \forall \mathbf{u},\mathbf{v},\mathbf{w} \in V\,.$$

Then we have

$$L(\mathbf{v}) = \frac{1}{2}\int_{\Omega}\int_{0}^{1} a(t\mathbf{v};t\mathbf{v},\mathbf{v})dtd\mathbf{x} - (\mathbf{f},\mathbf{v})\,.$$

An equivalent form of (2.28)-(2.29) yields

$$T \in {}^{1}V, Dl(T,z-T) \geq 0 \quad \forall z \in^{1} V\,, \tag{2.30}$$

$$\mathbf{u} \in K, DL(\mathbf{u},\mathbf{v}-\mathbf{u}) \geq 0 \quad \forall \mathbf{v} \in K\,, \tag{2.31}$$

where $l(z)$ and $L(\mathbf{v})$ are defined above.

Since the bilinear form $b(T,z)$ is V-elliptic and bounded then the thermal part of the problem can be analysed as in the classical linear case, which means to minimize an equivalent quadratic functional over the space of virtual temperatures. The non-linear elastic part of the problem can be solved by the secant modules method (see e.g. Nečas, Hlaváček (1983), Nedoma (1998)).

The `secant modules method` consists in solving a sequence of variational inequalities of the form

$$\mathbf{u}_{n+1} \in K,\ a(\mathbf{u}_n;\mathbf{u}_{n+1},\mathbf{v}-\mathbf{u}_{n+1}) \geq (\mathbf{f},\mathbf{v}-\mathbf{u}_{n+1}),\quad n = 1,2,\ldots \tag{2.32}$$

where $\mathbf{u}_n$ is the $n-$th approximate solution of the problem studied.

Hence the problem studied leads to the solution of a sequence of variational inequalities with variable coefficients of the semi-coercive type of the form:

Let $\mathbf{u}_n \in K$, $n = 1,2,\ldots$ be such that

$$a(\mathbf{u}_n;\mathbf{u}_{n+1},\mathbf{v}-\mathbf{u}_{n+1}) \geq (\mathbf{f},\mathbf{v}-\mathbf{u}_{n+1}) \quad \forall \mathbf{v} \in K\,. \tag{2.33}$$

Numerical approximation of the problem:

Let the domain $\Omega \subset \mathbb{R}^N$, $N = 2(3)$, be triangulated. Then let the domain $\overline{\Omega} = \Omega \cup \partial\Omega$ be divided into a system of m triangles T_h in the 2D case and into a system of m tetrahedra in the 3D case, generating triangulation $\mathcal{T}_h$ such that $\overline{\Omega} = \bigcup_{i=1}^{m} T_{hi}$ and such that two neighbouring triangles have only a vertex or an entire side common in the 2D case, and/or that two neighbouring tetrahedra have only a vertex or an entire edge or an entire face common in the 3D case. Let $h = \max_{1\leq i\leq m}(\text{diam } T_{hi})$ and let a family of triangulation $\{\mathcal{T}_h\}$, $h \to 0_+$, be regular in the standard sense. We further assume that sets $\overline{\Gamma}_u \cap \overline{\Gamma}_\tau, \overline{\Gamma}_u \cap \overline{\Gamma}_c, \overline{\Gamma}_\tau \cap \overline{\Gamma}_c$ coincide with vertices or edges of $\mathcal{T}_h$. Let

$$\begin{aligned}
{}^{1}V_h &= \{z \mid z \in C(\Omega),\ z\,|_{T_h} \in P_1,\ z = T_1 \text{ on } \Gamma_\tau \cup\ {}^{2}\Gamma_u\,,\\
V_h &= \{\mathbf{v} \mid \mathbf{v} \in [C(\Omega)]^N, \mathbf{v}\,|_{T_h} \in [P_1]^N, \mathbf{v} = \mathbf{u}_0 \text{ on } \Gamma_u \ \ \forall T_h \in \mathcal{T}_h\}\,,
\end{aligned}$$

where P_1 is the space of all linear polynomials, and

$$K_h = \left\{ \mathbf{v} \mid \mathbf{v} \in V_h, v_n^k - v_n^l \le 0 \text{ on } \bigcup_{k,l} \Gamma_c^{kl} \right\} = K \cap V_h \, .$$

We see that K_h is a convex and closed subset of V_h $\forall h$. Then using the FEM-secant modules method the problem leads to a sequence of approximate problems of variational inequalities with variable coefficients of the semi-coercive type of the form:

find $\mathbf{u}_{n+1}^h \in K_h$, $n = 1, 2, \dots$ such that

$$a(\mathbf{u}_n^h; \mathbf{u}_{n+1}^h, \mathbf{v} - \mathbf{u}_{n+1}^h) \ge (\mathbf{f}^h, \mathbf{v} - \mathbf{u}_{n+1}^h) \quad \forall \mathbf{v} \in K_h \, . \tag{2.34}$$

The analysis of such problems is parallel to that of the FEM approximation of variational inequalities in linear elasticity (see e.g. Hlaváček et al. (1988), Nedoma (1998), Hlaváček, Nedoma (2000)), as the variational inequality problem (2.34) represents a system of variational inequalities in the theory of linear elasticity where the elastic coefficients c_{ijkl} are replaced by variable coefficients $c_{ijkl}^* = c_{ijkl}^*(\mathbf{u}_n^h) = \lambda A^{\lambda-1}(e_{ij}(\mathbf{u}_n^h))c_{ijkl}(\mathbf{u}_n^h)$. Similarly as in the linear case it can be found that

$$\| \mathbf{u}_{n+1}^h - \mathbf{u}_n^h \|_1 \to 0 \quad \text{for} \;\; h \to 0 \tag{2.35}$$

and for the thermal part of the problem

$$\| T - T_h \|_1 \to 0 \quad \text{for} \;\; h \to 0 \, . \tag{2.36}$$

The algorithms are modifications of those used for linear heat equation and in the theory of contact problems in linear elasticity, which have been discussed e.g. in Nečas, Hlaváček (1981), Nedoma (1998) and which is shortly discussed in the next section.

2.2 Coupled Contact-Stefan Models

Introduction

In this part we will study dynamic contact problems in linear elasticity and thermo-elasticity describing geodynamic problems in R^N, $N = 2(3)$. The thermal parts of such problems are described by the so-called Stefan-like problems. In geomechanic problems such problems represent problems of recrystallization, namely near the contact boundary and evoked by the deformation of rocks and by the effect of the Coulombian friction.

We will deal with the following problem:

Let $\Omega = \bigcup_{\iota=1}^{s} \Omega^\iota \subset R^N$, $N = 2(3)$, be a smoothly bounded convex domain with boundary $\partial\Omega = \Gamma_u \cup \Gamma_\tau$, $\Gamma_u = \bigcup_{\iota=1}^{s} \Gamma_u$, $\Gamma_\tau = \bigcup_{\iota=1}^{s} \Gamma_\tau$, occupied by colliding bodies Ω^ι with boundaries $\partial\Omega^\iota = \Gamma_u^\iota \cup \Gamma_\tau^\iota \cup \Gamma_c^\iota$, $\Gamma_c^\iota = \bigcup_{k,l;k\neq l} \Gamma_c^{kl}$, $\Gamma_c^{kl} = \overline{\Omega}^k \cap \overline{\Omega}^l$, $k \neq l$. Let the stress-strain relation and the small strain tensor be defined by

$$\tau_{ij} = c_{ijkl} e_{kl}(\mathbf{u}) - \beta_{ij}(T - T_0), \quad e_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \quad i, j = 1, 2, (3) \, , \tag{2.37}$$

where $\beta_{ij} \in C^1(\overline{\Omega})$, $\beta_{ij} = \beta_{ji}$, is a coefficient of linear thermal expansion, $T_0(\mathbf{x}) \in H^1(\Omega)$ is the initial temperature at $t = t_0$, and coefficients of elasticity $c_{ijkl} \in C^1(\overline{\Omega})$ satisfy

$$c_{ijkl} = c_{jikl} = c_{klij}, \; c_{ijkl} e_{ij} e_{kl} \ge c_0 e_{ij} e_{ij}, \; c_0 = \text{const.} > 0, \;\; \forall e_{ij} = e_{ji}, \; \forall \mathbf{x} \in \overline{\Omega} \, . \tag{2.38}$$

Let ρ be the density, κ the specific heat about which we assume that it is a function of temperature T and pressure p, and function W represents thermal sources. Let $\overline{I} = \langle t_0, t_1 \rangle$, let $\mathbf{n}$ be the unit outward normal to $\Gamma_c = \cup \Gamma_c^{kl}$ related to Ω^k, $u_n = u_i n_i$ and $\mathbf{u}_t = \mathbf{u} - u_n \mathbf{n}$ be the normal and tangential components of the displacement vector $\mathbf{u}$, respectively; let $\tau_n(\mathbf{u})$ and $\tau_t(\mathbf{u})$ be the normal and tangential components of the stress vector $\tau(\mathbf{u}) = (\tau_i(\mathbf{u}))$, $\tau_i(\mathbf{u}) = \tau_{ij}(\mathbf{u}) n_j$ and $\boldsymbol{\tau}_t = \boldsymbol{\tau} - \tau_n \mathbf{n}$, τ_{ij} be the stress tensor and F_c^{kl} the coefficient of Coulombian friction. Using the usual Kirchhoff transformation $\Theta = \int_{T_0}^{T(\mathbf{x},t)} \kappa(\mathbf{x}, t, p, \xi) d\xi$, we have the following problem:

Problem ($\mathbf{P}_c$): Find a pair of functions $(\Theta, \mathbf{u})$ satisfying

$$\rho c \frac{\partial \Theta}{\partial t} + \rho \beta_{ij} \Theta_0 e_{ij}(\dot{\mathbf{u}}) - \Delta\Theta = W \text{ for a.e. } (\mathbf{x}, t) \in \Omega \times I, \quad i,j = 1,2,(3)\,, \tag{2.39}$$

$$\frac{\partial}{\partial x_j}[c_{ijkl} e_{kl}(\mathbf{u}) - \beta_{ij}(\Theta - \Theta_0)] - f_i = 0 \text{ for a.e. } (\mathbf{x}, t) \in \Omega \times I, \quad i,j,k,l = 1,2,(3)\,, \tag{2.40}$$

and the following conditions for all $t \in I$

$$\Theta = 0,\ \tau_{ij} n_j = P_i,\ (\mathbf{x}, t) \in \Gamma_\tau\,, \tag{2.41}$$

$$\Theta = 0,\ \mathbf{u} = 0,\ (\mathbf{x}, t) \in \Gamma_u, \tag{2.42}$$

$$\Theta^k = \Theta^l,\ \partial\Theta/\partial n|_{(k)} = \partial\Theta/\partial n|_{(l)},\ (\mathbf{x}, t) \in \bigcup_{kl} \Gamma_c^{kl}\,, \tag{2.43}$$

$$u_n^k - u_n^l \le 0,\ \tau_n^{kl} \equiv \tau_n^k = -\tau_n^l \le 0,\ \tau_n^{kl}(u_n^k - u_n^k) = 0\,, \tag{2.44}$$

$$\begin{aligned} &\text{if } u_n^k - u_n^l = 0 \text{ then } |\boldsymbol{\tau}_t^{kl}| \le g_c^{kl} \text{ and} \\ &\text{if } |\boldsymbol{\tau}_t^{kl}| < g_c^{kl} \text{ then } \mathbf{u}_t^k - \mathbf{u}_t^l = 0\,, \\ &\text{if } |\boldsymbol{\tau}_t^{kl}| = g_c^{kl} \text{ then } \exists \lambda \ge 0 \text{ such that } \mathbf{u}_t^k - \mathbf{u}_t^l = -\lambda \boldsymbol{\tau}_t^{kl} \text{ on } \cup \Gamma_c^{kl}\,. \end{aligned} \tag{2.45}$$

Let $R^m(t)$ be the phase change boundaries of two different phases at time. These boundaries divide the domain Ω into domains Ω_S^m and Ω_L^m. On $R^m(t)$ the following conditions are given

$$\Theta_S^m = \Theta_L^m = \Theta_R^m,\ \partial\Theta/\partial x_j \nu_j|_S^m - \partial\Theta/\partial x_j \nu_j|_L^m = -\rho^m L^m v_\nu^m\,, \tag{2.46}$$

where Θ_R^m is the temperature of the phase transition, Θ_S^m, Θ_L^m are the temperatures of solid and recrystalized phases at the phase change boundary $R^m(t)$, ν^m is the unit normal to $R^m(t)$ pointing towards Ω_S^m, v_ν^m is the speed of $R^m(t)$ along ν^m, and L^m is the latent heat, c_S^m, c_L^m, ρ_S^m, ρ_L^m are specific heats and densities in both phases and $\rho_S^m = \rho_L^m = \rho^m$ on $R^m(t)$. Moreover, the initial condition

$$\Theta(\mathbf{x}, t_0) = \Theta_0(\mathbf{x}) \tag{2.47}$$

is given.

In a similar way, as can be found in the variational inequality approach in enthalpy formulation, we define a generalized enthalpy $H(\Theta)$ as the subdifferential of the functional $\Phi(\Theta)$ as

$$\Phi(\Theta) = \frac{1}{2}\rho_L^m c_L^m (\Theta - \Theta_R^m)_+^2 + \frac{1}{2}\rho_S^m c_S^m (\Theta - \Theta_R^m)_-^2 + \rho^m L^m (\Theta - \Theta_R^m)_+\,, \tag{2.48}$$

i.e. $\partial\Phi(.) : R \to R$ is represented by a monotonically increasing multi-valued function of temperature with a jump discontinuity of the phase change temperature Θ_R^m. Then (2.39), (2.41), (2.42), (2.43), (2.46), (2.47) yield

$$\frac{\partial H(\Theta)}{\partial t} + \rho \beta_{ij} \Theta_0 e_{ij}(\dot{\mathbf{u}}) = \Delta\Theta + W,\ (\mathbf{x}, t) \in \Omega \times I\,, \tag{2.49}$$

$$\Theta(\mathbf{x}, t) = 0,\ \text{on } \Gamma_u \cup \Gamma_\tau,\ \ \forall t\,, \tag{2.50}$$

$$H(\mathbf{x}, t_0) = H_0(\mathbf{x})\,. \tag{2.51}$$

It can be shown that $\rho\beta_{ij}\Theta_0 e_{ij}(\dot{\mathbf{u}}) \in L^2(\Omega)$ $\left(\dot{\mathbf{u}} = \mathbf{u}_t = \frac{\partial \mathbf{u}}{\partial t}\right)$ and $\frac{\partial}{\partial x_j}(\beta_{ij}(\Theta - \Theta_0)) \in L^2(\Omega)$ have the meaning of thermal sources and body forces (see Nedoma (1987), (1998)). Let us define the space of virtual temperatures and displacements and the set of admissible displacements by

$$\begin{aligned} {}^1V &= \{z | z \in H^1(\Omega),\ z = 0 \text{ on } \Gamma_u \cup \Gamma_\tau\}\,, \\ V &= \{\mathbf{v} | \mathbf{v} \in [H^1(\Omega)]^N,\ \mathbf{v} = 0 \text{ on } \Gamma_u\}\,, \\ K &= \left\{ \mathbf{v} | \mathbf{v} \in V,\ v_n^k - v_n^l \le 0 \text{ on } \bigcup_{k,l,k \ne l} \Gamma_c^{kl} \right\}. \end{aligned}$$

Multiplying (2.49) by $w - \Theta_t$ and (2.40) by $v_i - u_{it}$, integrating over Ω, using the Green theorem and the boundary conditions and integrating over time, we obtain the following variational problem (we denote by $\dot{f} = f_t = \frac{\partial f}{\partial t}$):

Problem ($\mathbf{P}_{cs}$): Find Θ, $\Theta_t \in L^2(I;H^1(\Omega))$, $\mathbf{u} \in L^2(I;K)$, $\mathbf{u}_t \in L^2(I;H^1(\Omega))$ satisfying

$$\int_{t_0}^{t}[(H(\Theta_t), w-\Theta_t)+b(T,w-\Theta_t)+j(w)-j(\Theta_t)]d\tau \geq \int_{t_0}^{t}(W,w-\Theta_t)d\tau - \int_{t_0}^{t}\rho\beta_{ij}\Theta_0 e_{ij}(\dot{\mathbf{u}})(w-\Theta_t)d\tau,$$
$$\forall w \in L^2(I;H^1(\Omega)),\ t\in (t_0,t_1\rangle\,, \tag{2.52}$$
$$\int_{t_0}^{t_1}[a(\mathbf{u},\mathbf{v}-\mathbf{u}_t)+j_{gn}(\mathbf{v})-j_{gn}(\mathbf{u}_t)]\,d\tau \geq$$
$$\int_{t_0}^{t}\left[\int_\Omega f_i(v_i-u_{it})d\mathbf{x}+\int_{\Gamma_\tau}P_i(v_i-u_{it})ds+\int_\Omega\left(\frac{\partial}{\partial x_j}(\beta_{ij}(\Theta-\Theta_0)\right)(v_i-u_{it})d\mathbf{x}\right]d\tau \equiv$$
$$\equiv \int_{t_0}^{t}S(\mathbf{v}-\mathbf{u}_t)d\tau\ \ \forall \mathbf{v}\in L^\infty(I;K),\ t\in(t_0,t_1\rangle \tag{2.53}$$

and

$$\Theta(\mathbf{x},t_0)=\Theta_0(\mathbf{x})\,, \tag{2.54}$$

where $W-\rho\beta_{ij}\Theta_0 e_{ij}(\dot{\mathbf{u}}) \in L^2(I;L^2(\Omega))$, $(\mathbf{u},\mathbf{v})=\int_\Omega \mathbf{u}\mathbf{v}d\mathbf{x}$, $P_i \in L^2(I;L^2(\Gamma_\tau))$, $g_c^{kl}(\mathbf{x}) \in L^\infty(\Gamma_c^{kl})$, $g_c^{kl} \geq 0$ a.e. on Γ_c^{kl}, $f_i \in L^2(I;L^2(\Omega))$, $b(\Theta,w)=\int_\Omega$ grad Θ grad $wd\mathbf{x}$, $j(z)=\int_\Omega \Phi(z)d\mathbf{x}$, $(Q,w)=\int_\Omega Wwd\mathbf{x} - \int_\Omega \rho\beta_{ij}\Theta_0 e_{ij}(\dot{\mathbf{u}})wd\mathbf{x} \equiv s(w)$, $a(\mathbf{u},\mathbf{v})=\int_\Omega c_{ijkl}\mathbf{e}_{ij}(\mathbf{u})e_{kl}(\mathbf{v})d\mathbf{x}$, $S(\mathbf{v})=\int_\Omega f_i v_i d\mathbf{x}+\int_{\Gamma_\tau}P_i v_i d\mathbf{x}+\int_\Omega \frac{\partial}{\partial x_j}{}_j(\beta_{ij})\Theta - \Theta_0))v_i d\mathbf{x}$, $j_{gn}(\mathbf{v})=\int_{\cup\Gamma_c^{kl}} g_c^{kl}|\mathbf{v}_t^k-\mathbf{v}_t^l|ds$.

The above formulations represent parabolic and elliptic (with time t as a parameter) variational inequalities where the first inequality is a parabolic variational inequality of the second order introduced and discussed by Duvaut, Lions (1972), Brezis (1972) and Barbu (1976), and the second one is an elliptic variational inequality with time as a parameter obtained from the variational formulation of contact problems (Nedoma (1998)). Under certain assumptions there exists a unique pair of weak solutions $(\Theta,\mathbf{u})$ of problem (P_{cs}).

Numerical Solution

Let us put $\frac{\partial H(\Theta)}{\partial t}=k^{-1}(H(\Theta^{n+1})-H(\Theta^n))$, $\Theta^n=\Theta(\mathbf{x},nk)$, then Eq. (2.49) yields

$$H(\Theta^{n+1})-k\Delta\Theta^{n+1}+k\rho\beta_{ij}\Theta_0 e_{ij}(\mathbf{u}_t^n)=H(\Theta^n)+kW^{n+1}\,,$$

where $W^{n+1}=k^{-1}\int_{nk}^{(n+1)k}W(\tau)d\tau$, $\mathbf{u}_t^n=k^{-1}(\mathbf{u}^n-\mathbf{u}^{n-1})$.

To solve the Stefan part of the problem, the formulation in the form of a generalized non-linear boundary value problem discussed in Barbu (1976) and Glowinski (1979) will be used.

This differential equation is discontinuous, as Θ passes through Θ_R^m, and hence, together with the above boundary conditions, it represents a free boundary problem. For simplicity reasons we put $\Theta \equiv \Theta^{n+1}$, $\mathbf{u} \equiv \mathbf{u}^{n+1}$, $Q=H(\Theta^n)+kW^{n+1}+\alpha\Theta_R$, $\alpha\Theta+\partial\Phi(\Theta)\equiv H(\Theta)+\alpha\Theta_R$, where $0<\alpha\leq \min(\rho_S^m c_S^m,\rho_L^m c_L^m)$, $\alpha_i=\rho_i^m c_i^m-\alpha$, $i=S$ or L, respectively. Then we have to solve the following problem:

$$\alpha\Theta-k\Delta\Theta+\partial\Phi(\Theta)+k\rho\Theta_0\beta_{ij}e_{ij}(\mathbf{u}_t) \ni Q(\mathbf{x}) \text{ a.e. } \mathbf{x}\in\Omega,\ t \text{ fixed.}, \tag{2.55}$$
$$\Theta=0 \text{ a.e. } \mathbf{x}\in\partial\Omega\,. \tag{2.56}$$

Let us define the space of virtual temperatures as

$${}^1V=\{z|z\in H^1(\Omega), z=0 \text{ on } \partial\Omega\}\,,$$

and the space of virtual displacements V and the set of admissible displacement K as above. Then the variational (weak) formulation of the problem is the following:

Find a pair of functions $(\Theta,\mathbf{u})$, $\Theta\in^1 V$, $\mathbf{u}\in K$, such that

$$\alpha(\Theta, z-\Theta) + kb(\Theta, z-\Theta) + j(z) - j(\Theta) \geq s(z-\Theta) \;\; \forall z \in^1 V\,, \tag{2.57}$$
$$a(\mathbf{u}, \mathbf{v}-\mathbf{u}) + j_{gn}(\mathbf{v}) - j_{gn}(\mathbf{u}) \geq S(\mathbf{v}-\mathbf{u}) \;\; \forall \mathbf{v} \in K\,, \tag{2.58}$$

where $s(z) = (Q, z) - (k\rho\Theta_0\beta_{ij}e_{ij}(\mathbf{u}_t), z)$ or in an equivalent form:

find $(\Theta, \mathbf{u})$, $\Theta \in^1 V$, $\mathbf{u} \in K$ such that

$$l(\Theta) \leq l(z) \;\; \forall z \in^1 V\,, \tag{2.59}$$
$$L(\mathbf{u}) \leq L(\mathbf{v}) \;\; \forall \mathbf{v} \in K\,. \tag{2.60}$$

Problem (2.57) is equivalent to that of finding $\Theta \in^1 V$ such that $l(\Theta) = \inf_{z \in^1 V}\{l(z) = \frac{1}{2}\alpha(z,z) + \frac{1}{2}kb(z,z) + j(z) - s(z)\}$. The main difficulty represents the non-differentiable functional $j(\mathbf{v})$. Since $j(\mathbf{v})$ can be approximated as $j_{gn}(\mathbf{v}) = \sup_{\mu_{kl} \in \Lambda} \int_{\cup\Gamma_c^{kl}} \mu^{kl} g_c^{kl}(\mathbf{v}_t^k - \mathbf{v}_t^l)ds$, where μ^{kl} are Lagrangian multipliers and $\Lambda = \{\mu^{kl} \in L^2(\Gamma_c^{kl}) \mid\mid \mu^{kl} \mid\leq 1$ a.e. on $\cup\Gamma_c^{kl}\}$, then $\inf_{\mathbf{v}\in K} L(\mathbf{v}) = \inf_{\mathbf{v}\in K}\sup_{\mu\in\Lambda} L(\mathbf{v}, \mu)$, where $L(\mathbf{v}, \mu)$ is a Lagrangian defined by $L(\mathbf{v}, \mu) = L_0(\mathbf{v}) + \int_{\cup\Gamma_c^{kl}} \mu^{kl} g_c^{kl}(\mathbf{v}_t^k - \mathbf{v}_t^l)ds$, $L_0(\mathbf{v}) = \frac{1}{2}a(\mathbf{v}, \mathbf{v}) - S(\mathbf{v})$.

For the finite element approximation we will assume that $N = 2$ and that Ω is polygonal. Let domain Ω be covered by a finite number of triangles $\underline{T}_h$, forming a triangulation $\mathcal{T}_h$ and let the end points $\overline{\Gamma}_u \cap \overline{\Gamma}_\tau, \overline{\Gamma}_u \cap \overline{\Gamma}_c, \overline{\Gamma}_c \cap \overline{\Gamma}_\tau$ coincide with the vertices of $\underline{T}_h$. Let $h_0 > 0$ and let us assume that a family of triangulations $\{\mathcal{T}_h\}$, $0 < h \leq h_0$, is regular. Let us define the spaces of finite elements

$$\begin{aligned} {}^1V_h &= \{z | z \in C(\Omega),\; z|_{\underline{T}_h} \in P_1,\; z = 0 \text{ on } \partial\Omega,\; \forall \underline{T}_h \in \mathcal{T}_h\}\,, \\ V_h &= \{\mathbf{v} | \mathbf{v} \in [C(\Omega)]^2,\; \mathbf{v}|_{\underline{T}_h} \in [P_1]^2,\; \mathbf{v} = 0 \text{ on } \Gamma_u,\; \forall \underline{T}_h \in \mathcal{T}_h\}\,, \end{aligned}$$

where P_1 is the space of all linear polynomials,

$$K_h = \{\mathbf{v} | \mathbf{v} \in V_h,\; v_n^k - v_n^l \leq 0 \text{ on } \cup\Gamma_c^{kl}\}$$

be the finite element approximation of the set of admissible displacements. Let us denote by $\|\cdot\|_{k,N}$ the norm in $[H^k(\Omega)]^N$, k, N being integers.

A pair of functions $(\Theta_h, \mathbf{u}_h)$ is the finite element approximation of the problem if

$$\alpha(\Theta_h, z_h - \Theta_h) + kb(\Theta_h, z_h - \Theta_h) + j(z_h) - j(\Theta_h) \geq s(z_h - \Theta_h) \quad \forall z_h \in^1 V_h\,, \tag{2.61}$$
$$a(\mathbf{u}_h, \mathbf{v}_h - \mathbf{u}_h) + j_{gn}(\mathbf{v}_h) - j_{gn}(\mathbf{u}_h) \geq S(\mathbf{v}_h - \mathbf{u}_h) \quad \forall \mathbf{v}_h \in K_h \tag{2.62}$$

or in an equivalent form in which we will assume that nodes of triangulation $\mathcal{T}_h$ lying on the contact boundary $\cup\Gamma_c^{kl}$ are coincided with the nodes consistent with the boundary of supp g_c^{kl} in $\cup\Gamma_c^{kl}$ (in general these systems of points need not coincide, see Hlaváček et al. (1988)):

find $\Theta_h \in^1 V_h$ and a saddle point $(\mathbf{u}_h, \lambda_h) \in K_h \times \Lambda_h$ such that

$$l_h(\Theta_h) \leq l_h(z_h) \quad \forall z_h \in^1 V_h\,, \tag{2.63}$$
$$L_h(\mathbf{u}_h, \lambda_h) \leq L_h(\mathbf{u}_h, \mu_h) \leq L_h(\mathbf{v}_h, \mu_h) \quad \forall(\mathbf{v}_h, \mu_h) \in K_h \times \Lambda_h\,, \tag{2.64}$$

where $L_h(\mathbf{v}_h, \mu_h)$ represents the finite element approximation of the Lagrangian $L(\mathbf{v}, \mu)$ and $\Lambda_h = \cup\{\mu_h^{kl} | \mu_h^{kl} \in L^2(\Gamma_{ch}^{kl}),\; |\mu_h^{kl}| \leq 1$ a.e. on $\cup\Gamma_{ch}^{kl}\}$.

The algorithm of the problem is equivalent to that of finding $(\Theta_h, \mathbf{u}_h)$, $\Theta_h \in^1 V_h$, $\mathbf{u}_h \in K_h$ such that

$$l_h(\Theta_h) = \min_{z\in {}^1V_h} \left\{ l_h(z) = \frac{1}{2}\alpha(z,z)_h + 1/2kb_h(z,z) + j_h(z) - s(z)_h \right\}, \quad (2.65)$$

$$L_h(\mathbf{u}_h) = \min_{\mathbf{v}\in K_h} \sup_{\mu\in\Lambda_h} \left\{ L(\mathbf{v},\mu) = L_0(\mathbf{v}) + \int_{\cup\Gamma_c^{kl}} \mu^{kl} g_c^{kl}(\mathbf{v}_t^k - \mathbf{v}_t^l)ds \right\}. \quad (2.66)$$

Numerically (2.65) leads at every time level to minimizing the functional $l_h(z) = \frac{1}{2}z^T Bz - d^T z + \Phi(z)$, where $B = \alpha I + kB_0$, B_0 represents the FE approximation of $b_h(.,.)$, $\Phi(z) = \sum_{i=1}^{n}(\Phi(z_i))$, d^T corresponds to thermal sources, one part of which is generated by the dissipative thermal energy. Let $(z_i)_{i=1}^n$ be the basis of space ${}^1V_h$. Then every element of ${}^1V_h$ can be found as a linear combination of the basis $\{z_i\}$, similarly for Θ and Q. Then, in the usual way, we obtain a non-linear system of algebraic equations $Bz - d + \partial\Phi(z) = 0$, where $\partial\Phi(z) = MH(z)$ is the subdifferential of the functional $\Phi(z)$, $\partial\Phi(z) = (\partial\Phi(z_1),\ldots,\partial\Phi(z_n))$, $M = \left\{\int_\Omega z_i z_j d\mathbf{x}\right\}_{i,j=1}^n$. Then, if the matrix M and B are positive definite, the functional l_h has a Gâteaux derivative and is monotone on R^n. Then the functional l^h is uniformly convex on R^n and, therefore, a minimizer of the Stefan part of the problem exists.

Numerically (2.66) leads to numerical approximation of a saddle point. By an approximate saddle point is meant a point $(\mathbf{u}_{sh},\lambda_h) \in K_h \times \Lambda \subset K \times \Lambda$ of a Lagrangian L on $K_h \times \Lambda_h$, if a saddle point $(\mathbf{u}_s,\lambda) \in K \times \Lambda$ exists and if $L(\mathbf{u}_{sh},\mu_h) \le L(\mathbf{u}_{sh},\lambda_h) \le L(\mathbf{v},\lambda_h)$ holds for all pairs of functions $(\mathbf{v}_h,\mu) \in K_h \times \Lambda$. For a numerical solution of this problem the Uzawa's or Arrow-Hurwicz's algorithms can be used.

In the case of the Uzawa's algorithm we assume that $\lambda_h^0 \in \Lambda$ be given ($\lambda_h^0 \equiv 0$). Let $\lambda_h^i \in \Lambda$ be known. Then we find $\mathbf{u}_{hi} \in K_h$ by $\min_{\mathbf{v}\in\mathbf{K}_h}\left\{L_0(\mathbf{v}) + \int_{\cup\Gamma_c^{kl}} \lambda_h^{kl} g_c^{kl}(\mathbf{v}_t^k - \mathbf{v}_t^l)ds\right\}$ and then find $\lambda_h^{i+1,kl} = P(\lambda_h^{i,kl} + \rho_i g_c^{kl}((u_{hi}^k)_t - (u_{hi}^l)_t)$, where P is a projection $P : L^2(\Gamma_c^{kl}) \to \Lambda$ and $0 \le \rho_1 \le \rho_i \le \rho_2, \rho_1, \rho_2$ are sufficiently small numbers following from the convergence theorem of Uzawa's algorithm (Ekeland,Temam (1976)). In every step of Uzawa's algorithm we minimize $\min_{\mathbf{v}\in K_h}\left\{L_0(\mathbf{v}) + \int_{\cup\Gamma_c^{kl}} \lambda_h^{kl} g_c^{kl}(\mathbf{v}_t^k - \mathbf{v}_t^l)ds\right\}$, which is equivalent to the problem of finding the minimum of the quadratic functional $f(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T C\mathbf{w} - \mathbf{b}^T\mathbf{w}$ with linear constraints $A\mathbf{w} \le \mathbf{d}$. Matrix C is positive (semi-)definite stiffness matrix, generated by $\frac{1}{2}a(\mathbf{v},\mathbf{v}), \mathbf{b}$ is the vector of body and surface forces as well as of the friction forces $\int_{\cup\Gamma_c^{kl}} \lambda_h^{i,kl} g_c^{kl}(\mathbf{v}_t^k - \mathbf{v}_t^l)ds$ and of an approximation of the thermal stresses $\int_\Omega \frac{\partial}{\partial x_j}(\beta_{ij}(\Theta^n - \Theta_0))d\mathbf{x}$ at the n-th time level. Matrix $A(m \times n)$ is the matrix of constraints generated by the condition of non-penetration $u_n^k - u_n^l \le 0$ on Γ_c^{kl} and therefore $\mathbf{d} \equiv \mathbf{0}$. For more details see e.g. Nedoma (1998), Kestřánek et al. (1997).

2.3 Conclusion

To construct a model of structures under the influence of critical conditions, like the high level radiactive waste repository, we must take into account the influence of global tectonics onto the local area, where the critical structures will be built as well as the influence of the resulting local geomechanic processes on the critical structure. Therefore, the main object will be a reconstruction of the geometry and geological structures of the global and local areas investigated as well as geodynamical and geomechanical processes taking place in these areas. To construct a model of global tectonics we have great difficulties with determination of the contact boundaries (deep faults, contact boundaries between the collided plates and blocks) and the geological structure of the investigated region as individual geologists have the different opinions of the studied problem. For such reason we compile all results attained by different specialists that we critically adapt and supply by recognitions of standpoints of simulation of geomechanic and geodynamic processes. Without any knowledge of a solution of an inverse contact-Stefan-like problem which, at present, represents an open mathematical problem our considerations based on the present knowledge are based on heuristic techniques only. Thus the models are based on the deep seismic sounding profiles, on the maps of the lower boundary of the lithoshpere, on the seismological observations, namely on detailed knowledge of the depths of earthquake foci, on the geothermal and geomechanical studies in the investigated region, on the analyses of thermal, gravity and other anomalies, on other geological and geophysical observations, experience with geophysical syntheses, on all knowledge about the topic and then compile all the found information together with the experience with construction of the previous models and results of inverse problems (if they exist as inverse coupled contact-Stefan-like problems represent an open mathematical problem). As a result we obtain modified maps of the lower boundary of the lithosphere as well as the geological structure of the investigated region. To construct a model of the local area we will progress in a similar way, i.e. it means to obtain maximum information about the local region. Moreover, we will use the results obtained from the previous steps representing the influences of global tectonics on the local area, like the distribution of the geothermal field, phase transition zones, fields of displacements, velocitities, stresses, analyses of thermal, gravity, and other anomalies. It is evident that the physical data obtained as well as the contact boundaries (deep faults, lower boundaries of the lithospheric plates, boundaries between geological blocks), the body and surface forces, thermal sources, etc. are uncertain. Thus mathematical models involve physical and geometrical data which cannot be determined uniquely but only in some intervals deteremined by the accuracy of our knowledge discussed above. For such problems the stochastic approach can be used (e.g. Holden et al. (1996)) or the method of reliable solution which is of a deterministic type (see Chleboun in the proceedings of the conference).

The methodology discussed in the previous subsections has been tested on a simple model problem assuming that the coefficients c_{ijkl} depend only on the coordinates only and $\lambda = 1$ and representing the obducting lithospheric plate (from the famous Grow's model of the Central Aleutians) being in collision with absolutely rigid foundations. Fig. 1 presents principal stresses at time $t^{\sim}10^5$ yrs in 10^9 Nm^{-2}. On the contact boundaries the bulged-out areas, corresponding to the condition of penetration (2.44) of Section 2.2 (i.e. the distribution of normal component of displacement vector), are illustrated. In next figures, representing a simple version of the geological structure of the region studied, the distribution of the temperature (in °K) (see Fig. 2) and the principal stresses in the global region, evoked by the thermal stresses (←→ – extension, →← – compression) also owing to an effect of the dissipative deformation energy changing into a heat (see Fig. 1b), are presented. Since the coefficient of thermal conductivity κ depends on the pressure, the phase-change free boundary is indicated. The model problem discussed shows the possible way for investigations global tectonic effects operating on the local region where the critical structure will be situated.

Acknowledgement:

This research was supported by the grant COPERNICUS-HIPERGEOS II-KIT No. 977006 and the grant of the Ministry of Education, Youth and Sports of the Czech Republic No OK-407.

Bibliography

[1] V.Barbu (1976). Nonlinear Semigroups and Differential Equations in Banach Spaces. Noordhoff, Leyden.

[2] H.Brezis (1971). Monotonicity Methods in Hilbert Spaces and Some Applications to Nonlinear Partial Differential Equations. In: E.H.Zarantonello (Ed.), Contribution to Nonlinear Functional Analysis, Academic Press, New York, 1971, 101-156.

[3] G.Duvaut,J.L.Lions (1976). Inequalities in Mechanics and Physics. Springer Vlg., Berlin, Heidelberg, New York.

[4] Ekeland I.,Temam R. (1976) Convex Analysis and Variational Problems. North-Holland Publ. Co., Amsterdam, Oxford.

[5] Freudenthal, A.M., Geiringer, H. (1958). The Mathematical Theories of the Inelastic Continuum. Handbuch der Physik-Encyclopedia of Physics, VII. Elasticity and Plasticity, Springer Vlg., Berlin, Göttingen, Heidelberg.

[6] Fung, Y.C. (1965). Generalized Hooke's Law. Foundations of Solid Mechanics. Prentice-Hall, N.J.

[7] Gajewski, H., Gröger, K, Zacharias,K. (1974). Nichtlineare Operatorgleichungen und Operatordifferentialgleichungen. Academie-Verlag, Berlin.

[8] R.Glowinski, (1979). Finite elements and variational inequalities. In: J.R. Whiteman (Ed.), The Mathematics of Finite Elements and Applications III, Academic Press, New York, 135-171.

[9] Haslinger, J., Hlaváček, I., Nečas, J. (1996). Numerical Methods for Unilateral Problems in Solid Mechanics. In: Handbook of Numerical Analysis. Vol.IV, Elsevier Science, Amsterdam, 313-486.

[10] Hlaváček, I., Haslinger, J., Nečas, J., Lovíšek, J. (1988). Solution of Variational Inequalities in Mechanics. Springer Vlg., New York.

[11] Hlaváček, I., Nedoma (2000). On a solution of a generalized semi-coercive contact problem in thermo-elasticity (submitted to Computer Methods in Applied Mechanics and Engineering).

[12] Holden, H, Øksendal, B., Ubøe, J., Zhang, T. (1996). Stochastic Partial Differential Equations. Birkhäuser, Boston, Basel, Berlin.

[13] Kestřánek Z., Dvořák J., Nedoma J., Iterative Solvers for Coupled Contact-Stefan-like Problems.In: World Congress on Scientific Computation, Modelling and Applied Mathematics. Proceedings. (Ed.: Sydow Achim) Vol.: 3. Computational Physics, Chemistry and Biology. - Berlin, Wissenschaft & Technik 1997, pp.467-471

[14] Kikuchi,N., Oden, J.T. (1988). Contact Problems in Elasticity: A Study of Variational Inequalities and Finite Element Methods. SIAM, Philadelphia.

[15] Nečas, J., Hlaváček, I. (1981). Mathematical Theory of Elastic and Elasto-Plastic Bodies: An Introduction. Elsevier, Amsterdam.

[16] Nečas, J., Hlaváček, I. (1983). Solution of Signorini's contact problem in the deformation theory of plasticity by secant modules method. Apl.Mat. 28(3),199-214.

[17] Nedoma, J. (1983). On one type of Signorini problem without friction in linear thermo-elasticity. Apl.Mat. 28(6), 393-407.

[18] Nedoma, J. (1987). On the Signorini problem with friction in linear thermo-elasticity. The quasi-coupled 2D-case. Apl. Mat. 32(3),186-199.

[19] Nedoma, J. (1994). Finite element analysis of contact problems in thermo-elasticity. The semi-coercive case. J.Comput.Appl.Math. 50,411-423.

[20] Nedoma, J. (1997). Finite element approximation of a coupled contact-Stefan-like problem arising from the time discretization in deformation theory of thermo-plasticity. J.Comput.Appl.Math. 82,313-334.

[21] Nedoma, J. (1998). Numerical Modelling in Applied Geodynamics. John Wiley&Sons, Chichester, New York, Weinheim, Brisbane, Singapore, Toronto.

[22] Nedoma,J., Hlaváček,I. (2001). Solution of a semi-coercive contact problem in a non-linear thermo-elastic rheology (submitted to Computer Methods in Applied Mechanics and Engineering).

[23] Panagiotopoulos, P.D. (1985). Inequality Problems in Mechanics and Applications. Convex and Non-Convex Energy Functions. Birkhäuser, Boston, Basel, Stuttgart.